Non-Markovian diffusion over a potential barrier in the presence of periodic time modulation

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(Received 24 August 2011; revised manuscript received 3 November 2011; published 22 November 2011)

The diffusive non-Markovian motion over a single-well potential barrier in the presence of a weak sinusoidal time modulation is studied. We found nonmonotonic dependence of the mean escape time from the barrier on a frequency of the periodic modulation that is analogous to the stochastic resonance phenomenon. The resonant increase of diffusion over the barrier occurs at the frequency inversely proportional to the mean first-passage time for the motion in the absence of the time modulation.

DOI: 10.1103/PhysRevE.84.051123 PACS number(s): 05.40.−a, 21.60.Ev, 21.10.Re, 24.30.Cz

I. INTRODUCTION

The response of complex nonlinear systems on periodic external fields may have features that are absent for linear systems. The very famous example of such features is the stochastic resonance phenomenon [1], when the response of the nonlinear system on the harmonic perturbation is resonantly activated under some optimal level of a noise. The resonant activation of the system occurs when the frequency of the modulation is near the Kramers escape rate of the transitions from one potential well to another. The stochastic resonance phenomenon has been found and studied in many physical systems, such as a ring laser [2], magnetic systems [3], optical bistable systems [4], and others (see, for example, the reviews [5] and [6]). Since its discovery in 1980, the phenomenon still attracts much interest. In this respect one can also mention the works of Refs. [7–9]. The prototype of the stochastic resonance studies is a model of overdamped motion between potential wells of the bistable system. The frequency of the transitions between wells is given by the famous Kramers rate, and the stochastic resonance is achieved when a frequency of an external periodic modulation is of the order of the Kramers rate.

In the present paper we study diffusion over a single-well potential barrier by the presence of a periodic time modulation. The diffusion over the barrier is generated by a colored noise whose statistical properties are related to the retarded dissipative properties of the nonlinear system. Following this conception, we address the problem of the stochastic resonance phenomenon to the many-body systems where the stochastic and damped features of the macroscopic modes of motion are related to each other through the fluctuation-dissipation theorem. It is also important that the macroscopic dynamics in the many-body systems may be essentially non-Markovian. The manifestation of the memory effects in the macroscopic dynamics is, for instance, the coexistence of the first- and zero-sound excitations in a Fermi liquid [10]. Here the memory effects appear because of the Fermi-surface distortion and depend on the relaxation time. Thus we are going to study a new aspect of the many-body dynamics, namely, how the correlation time of the colored noise [11–13], measuring the relative strength of memory effects in the motion of the system, influence the first-passage time distribution and escape rate over the barrier by the presence of periodic external field. In the case of a piecewise linear potential barrier, one can get an exact analytical result for the mean first-passage time problem [14–16]. The effect of a colored noise on the stochastic resonance has been also studied in Refs. [17–19]. In Ref. [19] it was shown that the stochastic resonance in overdamped bistable systems is suppressed by growth of a correlation time of the colored noise.

Note that for the dissipative dynamics, the colored noise has been investigated within different approaches. In this respect one can mention the dissipative diabatic model [20,21], linear response theory [22–24], and the generalized Langevin theory (see Refs. [25–27] and references therein). As is shown in Ref. [28], for the case of large-amplitude dynamics, the memory effect significantly influences the trajectory of motion as well as the dissipative characteristics at sufficiently large values of relaxation time. From the point of view of the fluctuation-dissipation theorem, it is of great interest to extend the investigation of the large-amplitude motion to the case of diffusive non-Markovian motion when the colored random force is taken into consideration. In the present paper we use the generalized Langevin theory [25,26] and apply such an approach to the study of the barrier overcome by the presence of the external drawing field.

The paper is organized as follows. In Sec. II we set a basic Langevin equation of motion for diffusive motion over a potential barrier in the presence of sinusoidal time modulation. In Sec. III A the unperturbed path of the model system is considered. The time-modulated diffusion is discussed in Sec. III B. Finally, the main conclusions of the paper are given in Sec. IV.

II. DIFFUSIVE MOTION OVER A POTENTIAL BARRIER

We start from a quite general Langevin formulation of the problem of diffusive overcoming of a potential barrier in the presence of a harmonic perturbation $V_{\text{ext}}(t) = \alpha \sin(\omega t)$. We restrict our analysis to the one-dimensional case. The generalization to the multidimensional collective dynamics can be obtained in a straightforward way (see, e.g., Refs. [25,29,30]). The one-dimensional and non-Markovian Langevin equation in the presence of a harmonic perturbation reads

$$M\ddot{q}(t) = -\frac{\partial E_{\text{pot}}}{\partial q} - \int_0^t \kappa(t-t')\dot{q}(t')dt' + \xi(t) + \alpha \sin(\omega t), \tag{1}$$

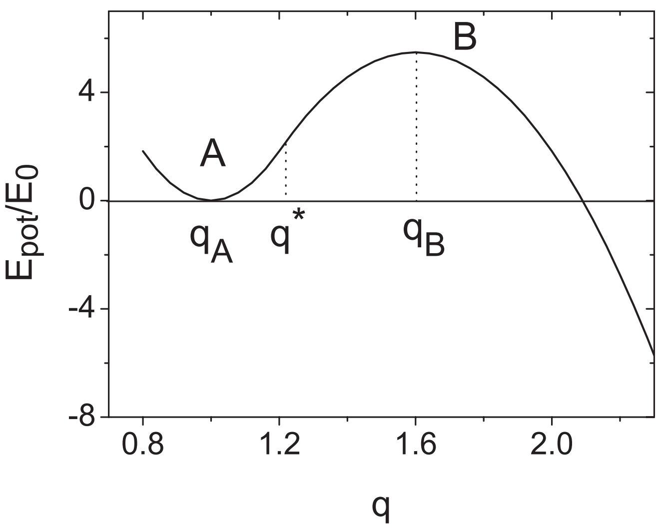

FIG. 1. Landscape of potential energy $E_{\rm pot}(q)$ of Eq. (2).

where q is the dimensionless coordinate, M is the mass, $\kappa(t-t')$ is the memory kernel, and $\xi(t)$ is the random force. The potential energy $E_{\rm pot}$ is schematically shown in Fig. 1 and presents a single-well barrier formed by a smoothing joining at $q=q^*$ of the potential minimum oscillator with the inverted oscillator:

$$E_{\rm pot} = \tfrac{1}{2}M\omega_A^2(q-q_A)^2, \quad q \leqslant q^*,$$
$$= E_{\rm pot,B} - \tfrac{1}{2}M\omega_B^2(q-q_B)^2, \quad q > q^*. \tag{2}$$

A noise term $\xi(t)$ in Eq. (1) is assumed to be Gaussian distributed with zero mean and correlation function related to a memory kernel $\kappa(t-t')$ of a retarded friction force:

$$\langle \xi(t)\,\xi(t')\rangle = T\,\kappa(t-t'). \tag{3}$$

Below we assume that the memory kernel is given by

$$\kappa(t-t') = \kappa_0 \exp\left(-\frac{|t-t'|}{\tau}\right), \tag{4}$$

where τ is a correlation time.

III. NUMERICAL CALCULATIONS

In the numerical calculations, we have measured all quantities of the dimension of energy in units of the temperature of the system $E_0 = T$, quantities of the dimension of time in units of $t_0 = \sqrt{M/T}$, and quantities of the dimension of frequency in units of $\omega_0 = \sqrt{T/M}$. For the system's parameters, q_A, q^*, q_B, ω_A, ω_B, $E_{\rm pot,B}$, and κ_0, we have adopted the values

$$q_A = 1, \quad q^* = 1.2, \quad q_B = 1.6, \quad \omega_A = 6.75,$$
$$\omega_B = 9.59, \quad E_{\rm pot,B} = 5.15, \quad \kappa_0 = 1920, \tag{5}$$

which are widely used under model diffusionlike studies of fission of highly excited atomic nuclei (see Ref. [28]).

A. Unperturbed diffusion over the barrier

In the beginning we investigated the non-Markovian diffusive dynamics for the infinitely slow ($\omega = 0$) modulation and calculated a first-passage time distribution. For that, the Langevin equation (1) was solved numerically by generating a bunch of the trajectories, all starting at the potential well (point A in Fig. 1) and having the initial velocities distributed according to the Maxwell-Boltzmann distribution. First we studied the diffusive dynamics (1)–(4) in terms of first-passage time distribution. Note that we apply here the first-passage time distribution to the simplest case of one-dimensional motion only. In a general case of many-dimensional dynamics, the transition path sampling technique [31] or the action method [32] can be used to sample the trajectories of collective motion in many-dimensional space.

In Fig. 2 the mean first-passage time is presented as a function of the correlation time τ. An increase of the mean first-passage time $t_{\rm mfpt}$ with the relaxation time τ means that memory effects in the Langevin dynamics (1) hinder the diffusion over the barrier. A non-monotonic growth of the mean first-passage time is caused by a transition (occurring at $\tau \approx 0.007$) from the nearly Markovian regime of the diffusion (1) to the regime where the memory effects are quite important. As far as the memory effects become stronger and stronger ($\tau \to \infty$), the value of $t_{\rm mfpt}$ reaches a finite limit. Here the hindrance of the escape over the barrier is caused by the renormalization of the ordinary conservative force in Eq. (1) that obtains an additional contribution from the time-retarded force:

$$-\kappa_0 \int_0^t \exp\left(-\frac{|t-t'|}{\tau}\right)\dot{q}(t')dt' \to -\kappa_0[q(t)-q_A],$$
$$\tau \to \infty. \tag{6}$$

In the opposite limit of quite small values of correlation time τ, the hindrance is exclusively due to an usual friction:

$$-\kappa_0 \int_0^t \exp\left(-\frac{|t-t'|}{\tau}\right)\dot{q}(t')dt' \to -\kappa_0\tau\dot{q}(t), \quad \tau \to 0. \tag{7}$$

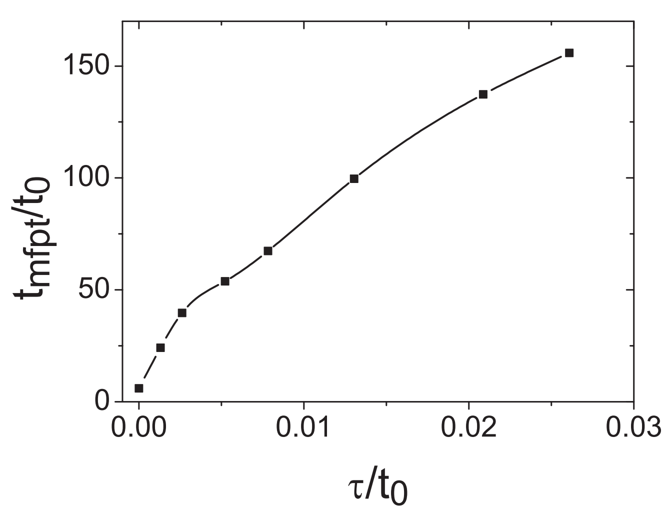

FIG. 2. Mean first-passage time $t_{\rm mfpt}$ of the non-Markovian diffusion process (1)–(4) vs the correlation time τ.

In the intermediate case, the hindrance is defined by both the friction and the additional elastic force,

$$-\kappa_0 \int_0^t \exp\left(- \frac{|t - t'|}{\tau} \right) \dot{q}(t')\, dt' = -\gamma(t,\tau)\, \dot{q}(t) - C(t,\tau)\, q(t), \qquad (8)$$

where the effective friction coefficient $\gamma(t,\tau)$ may be quite well approximated by

$$\gamma(t,\tau) \approx \frac{\kappa_0 \tau}{1 + (\kappa_0/M)\tau^2}, \quad t \gg \tau. \qquad (9)$$

The stiffness parameter $C(t,\tau)$ in Eq. (8) grows from 0 to κ_0 with the growth of τ.

Secondly, we measure the diffusion dynamics (1)–(4) through an escape rate $R(t)$ characteristics. The escape rate over the barrier is defined as

$$R(t) = -\frac{1}{P(t)} \frac{dP(t)}{dt}, \qquad (10)$$

where $P(t)$ is the survival probability, i.e., the probability of finding the system on the left from the top of the barrier up to time t:

$$P(t) = N(t)/N_0. \qquad (11)$$

Here $N(t)$ is the number of trajectories not reaching the top of the barrier up to time t and N_0 is the total number of trajectories involved in the calculations. In Fig. 3 is plotted the typical time behavior of the escape rate $R(t)$ for quite small, $\tau = 0.005$, and fairly large, $\tau = 0.026$, values of the correlation time.

It is seen from Fig. 3 that initially the escape is affected by transient effects, when the survival probability $P(t)$ deviates strongly from the exponential form. With time the escape process becomes more and more stationary, giving rise to the corresponding saturation rate $R(t)$ (10), establishing the quasistationary probability flow over the barrier. Qualitatively, one can describe the typical time evolution of the escape rate as

$$R(t) = R_0(1 - e^{-t/t_{\rm tran}}). \qquad (12)$$

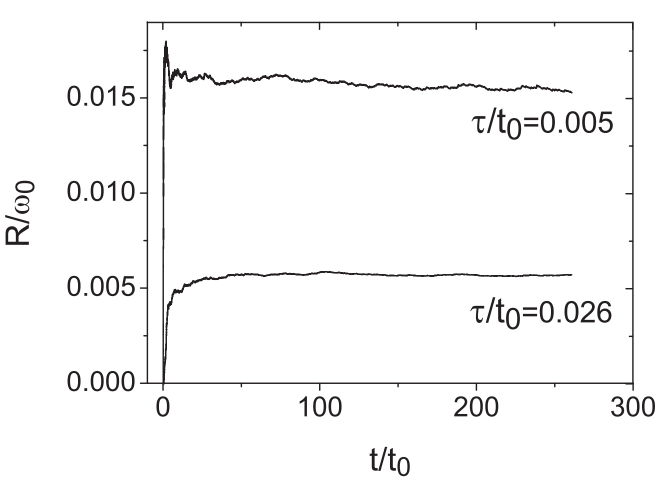

FIG. 3. Time dependence of the escape rate $R(t)$ (10) of the non-Markovian diffusion process (1)–(4) calculated for the cases of quite small $\tau = 0.005$ and fairly large $\tau = 0.026$ values of the correlation time.

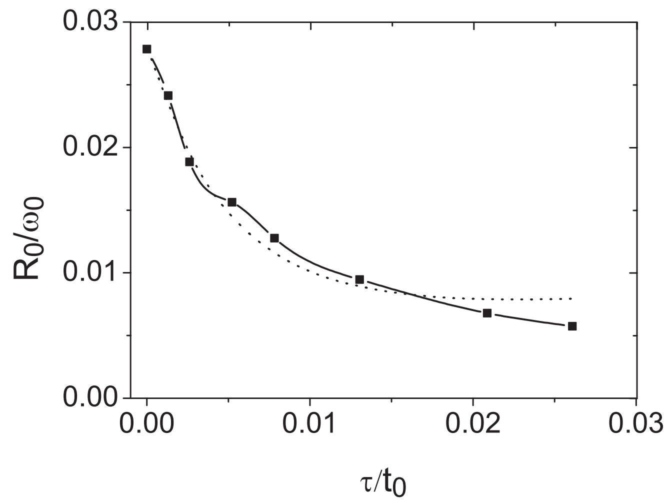

FIG. 4. Saturation value R_0 of the escape rate (10)–(12) vs the strength τ of the memory effects in the non-Markovian diffusion process (1)–(4). The dotted line represents the Kramers result (13) for the escape rate calculated with the τ-dependent friction coefficient of Eq. (9).

In both cases a duration of the transient period $t_{\rm tran}$ is almost the same ($t_{\rm tran} \approx 50$) for quite weak and fairly large memory effects in the diffusion process. However, a saturation value R_0 of the escape rate is significantly different because of the memory effect for the large values of the correlation time τ.

In Fig. 4 we showed how the value R_0 (12) depends on the size of the memory effects in the diffusive dynamics (1). The dotted line in Fig. 4 represents the famous Kramers result for the escape-rate value in a quasistationary regime [33],

$$R_{Kr} = \frac{\omega_A}{2\pi} \left(\sqrt{1 + \left[\frac{\gamma(\tau)}{2M\omega_B} \right]^2} - \frac{\gamma(\tau)}{2M\omega_B} \right) \exp\left(- \frac{E_{\rm pot,B}}{T} \right), \qquad (13)$$

where the τ-dependent friction coefficient $\gamma(\tau)$ is given by Eq. (9).

We see that the memory effects significantly suppress the value of the escape rate in the saturation regime of probability flow over the potential barrier. Initially (i.e., at relatively small values of the correlation time τ) the suppression is mainly caused by the growing role of the usual friction in the non-Markovian diffusion (1)–(4) [see also Eqs. (8) and (9)]. As seen from Fig. 4, in this case the escape rate at saturation R_0 (12) may be quite well approximated by the Kramers formula (13). On the other hand, at relatively large correlation times τ, the effect of the friction on the diffusion over the barrier is negligibly weak and the escape rate's suppression appears exclusively due to the additional conservative force [see Eq. (8)]. As a result, the stationary value of the escape rate deviates substantially from the Kramers escape rate (13) at the fairly strong memory effects in the diffusive motion across the barrier.

B. Diffusion over the barrier in the presence of a periodic modulation

Now we study the diffusion over the barrier (1)–(4) in the presence of the external harmonic force. We assume that

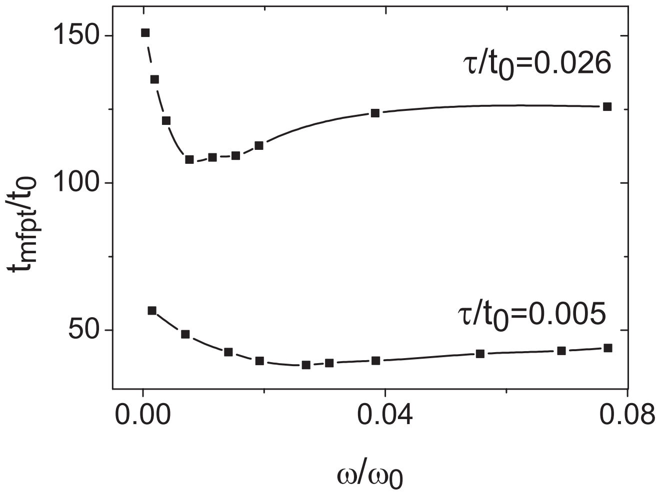

FIG. 5. Mean first-passage time $t_{\rm mfpt}$ of the non-Markovian diffusion process (1)–(4) is given as a function of the frequency ω of the harmonic time perturbation at two values of the correlation time $\tau = 0.005$ (lower curve) and $\tau = 0.026$ (upper curve).

the amplitude α of the force $\alpha\sin(\omega t)$ in Eq. (1) is so small ($\alpha = 0.05$) that reaching the top of the barrier is still caused exclusively by the diffusive nature of the process.

In Fig. 5 we calculated the typical dependencies of the mean first-passage time $t_{\rm mfpt}$ on the frequency ω of the external harmonic force. The calculations were performed for the weak, $\tau = 0.005$ (lower curve in Fig. 5), and strong, $\tau = 0.026$ (upper curve in Fig. 5), memory effect on the non-Markovian diffusive motion over the barrier.

In both cases the mean first-passage time $t_{\rm mfpt}$ nonmonotonically depends on the frequency of the perturbation that is characteristic of the stochastic resonance phenomenon observed in a number of different physical systems. From Fig. 5 one can conclude that diffusion over the potential barrier in the presence of the harmonic time perturbation is maximally accelerated at some definite resonant frequency $\omega_{\rm res}$ of the perturbation,

$$\omega_{\rm res} \approx \frac{1.5}{t_{\rm mfpt}(\omega = 0)} \tag{14}$$

(see also Figs. 2 and 4). In fact, the quantity $t_{\rm mfpt}(\omega = 0)$ presents the characteristic time scale for the diffusion dynamics (1). In the case of adiabatically slow time variations of the harmonic force, $\omega t_{\rm mfpt}(\omega = 0) \ll 1$ and $t < t_{\rm mfpt}$, one can approximately use $\alpha \cdot \sin(\omega t) \approx \alpha \cdot \omega t$ and the diffusion over the barrier is slightly accelerated. As a result of that, the mean first-passage time $t_{\rm mfpt}(\omega)$ is smaller than the corresponding unperturbed value $t_{\rm mfpt}(\omega = 0)$. The same feature is also observed at the fairly large modulation frequencies. Thus, in the case of $\omega t_{\rm mfpt}(\omega = 0) \gg 1$, the harmonic perturbation $\alpha\sin(\omega t)$ may be treated as a random noise term with zero mean value and variance α^2. Such a new stochastic term will lead to additional acceleration of the diffusion over the barrier.

The existence of the resonant regime (14) in the periodically modulated diffusion process (1) is even more clearly visible in the escape-rate characteristics of the process. We have plotted in Fig. 6 the time evolution of the escape rate (10) found for the resonant frequency $\omega_{\rm res}$ (14) (curve 1 in Fig. 6), the quite smaller frequency $\omega = \omega_{\rm res}/10$ (curve 2 in the Fig. 6), and the quite larger frequency $\omega = 10\omega_{\rm res}$ (curve 3 in Fig. 6) of the modulation.

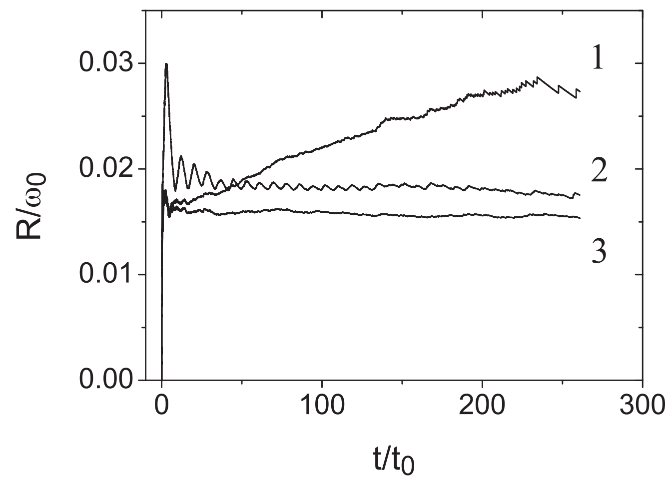

FIG. 6. Time dependencies of the escape rate R (10) for the periodically modulated diffusion over the barrier (1)–(4)) are shown at the resonant frequency $\omega_{\rm res}$ ((14) (curve 1), fairly smaller frequency $\omega = \omega_{\rm res}/10$ (curve 2), and quite larger frequency $\omega = 10\omega_{\rm res}$ (curve 3) of the periodic modulation. The dependencies were calculated for the memory time $\tau = 0.01$.

Again, at very slow ($\omega = \omega_{\rm res}/10$) and fast ($\omega = 10\omega_{\rm res}$) perturbations, the escape rate $R(t)$ looks very similar to the corresponding unperturbed value $R(t,\omega = 0)$ (compare Figs. 3 and 6). In other words, the initial transient period in the time evolution of the escape rate is followed by the stationary regime, when the escape subsequently saturates with time. Contrary to that, the escape rate shows complex time behavior as long as the periodic modulation occurs at the resonant frequency ($\omega = \omega_{\rm res}$) (see curve 1 in Fig. 6). This resonant regime of the modulated diffusion is essentially nonstationary when the system remains excited during quite long time. We checked such a feature for the larger number of trajectories and longer time intervals used to calculate the escape rate characteristics (10).

IV. CONCLUSIONS

In the present study we have investigated how model non-Markovian diffusion over the single-well parabolic barrier is affected by external periodic time modulation. We have calculated both the mean first-passage time $t_{\rm mfpt}$ and the escape rate $R(t)$ over the barrier. These two quantities have been found to be sensitive to the relative size of memory effects in the diffusive dynamics (1)–(4), measured by the correlation time τ. Thus we have demonstrated that the memory effects hinder the escape over the barrier (see Figs. 2 and 4). In contrast to the motion in the presence of usual friction force, the hindrance of the escape occurs due to the Markovian friction and additional conservative components (8) of the retarded time force in Eq. (1). Having calculated the mean first-passage time $t_{\rm mfpt}$ for different values of the frequency ω of the modulation, we have found that the sinusoidal perturbation accelerates the diffusion over the barrier (see Fig. 5). The maximal (resonant) acceleration is achieved at

$\omega = \omega_{\rm res}$, where $\omega_{\rm res}$ is inversely proportional to the mean first-passage time in the absence of the modulation (14). We have seen that a value of the resonant activation over the barrier $t_{\rm mfpt}(\omega = \omega_{\rm res})/t_{\rm mfpt}(\omega = 0)$ remains practically the same for the quite weak as well as for the fairly strong memory effects in the diffusive dynamics. It has been observed that the diffusive dynamics (1)–(4) in the resonant activation regime (14) has the peculiarity, reflecting in the complex time behavior of the escape rate $R(t)$ (see Fig. 6). Importantly, the absence of the escape rate's saturation with time implies the essentially transient character of the events of the first passage at the top of the potential barrier.

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